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NABESITE, $Na_2BeSi_4O_{10}•4H_2O$, A NEW MINERAL SPECIES FROM THE ILÍMAUSSAQ ALKALINE COMPLEX, SOUTH GREENLAND*

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ABSTRACT

Nabesite is found in complex tugtupite-bearing albitites on the Kvanefjeld Plateau, in the northwesternmost part of the Ilímaussaq alkaline complex, South Greenland. It occurs in cavities, covered with albite crystals, in association with gmelinite, neptunite, analcime, gonnardite, lovdarite, trona(?) and opal(?). Nabesite forms aggregates of thin platy crystals, in parallel or subparallel orientation, the individual crystals show the pinacoids {100}, {010}, {001}, and {111} and {111}, both sphenoids, and range in size from 0.05 × 0.5 × 0.5 to 0.2 × 5 × 5 mm. The mineral is colorless and transparent, it has a white streak, and the luster is vitreous. The Mohs hardness is 5–6, it is brittle and shows good cleavage on {110} and {001}, and the fracture is uneven. Nabesite is biaxial negative with n_α = 1.499(1), n_β = 1.507(1) and n_γ = 1.511(1), $2V_\alpha$ (measured) 65(5)°, $2V_\alpha$ (calculated) 70°, and has $X = a$, $Y = c$ and $Z = b$. D_{meas} = 2.16(2) g/cm^3, D_{calc} = 2.21 and 2.22 g/cm^3 for V derived from powder and single-crystal diffraction data, respectively. Data from EMP, SEM–EDS and results of the refinement of the crystal structure gave: Na_2O 13.8, K_2O 0.34, BeO 6.26, CaO 0.13, SiO_2 62.4, H_2O 18.05, total 100.98 wt%. The ideal formula is $Na_2BeSi_4O_{10}•4H_2O$. The strongest lines on the X-ray powder-diffraction pattern [*d* in Å(I)(*hkl*)] are: 6.11(80)(111), 5.97(100)(002), 3.09(70)(310), 3.06(50)(222) and 2.988(60)(311). The unit-cell parameters refined from the powder data are: *a* 9.722(1), *b* 10.142(1), *c* 12.030(1) Å, *V* 1186.2 Å^3. The structure was determined by single-crystal X-ray diffraction. Nabesite crystallizes in the orthorhombic space-group $P2_12_12_1$, *a* 9.748(1), *b* 10.133(1), *c* 11.954(2) Å, *V* 1180.8(2) Å^3, *Z* = 4. A total of 5704 unique reflections (at 293 K) gave a final *R*1 factor of 0.028 (*wR*2 = 0.078). The [SiO_4] tetrahedra form sheets consisting of a combination of 4- and 8-membered rings, which are interconnected *via* the [BeO_4] tetrahedra (a spiro-5 arrangement as secondary building unit) to form a framework. Channels house octahedrally coordinated sodium atoms and H_2O molecules with a well-established system of hydrogen bonds. Nabesite is a zeolite with a new type of framework; the framework density is 16.94 *T* / 1000 Å^3. Relationships to the crystal structure of weinebeneite are evident.

Keywords: nabesite, new mineral species, crystal structure, zeolite, Ilímaussaq alkaline complex, Greenland.

SOMMAIRE

On trouve la nabesite dans des venues complexes d'albitites à tugtupite sur le plateau de Kvanefjeld, à l'extrême nord-ouest du complexe alcalin d'Ilímaussaq, dans le sud du Groënland. Elle se présente en cavités, revouverte de cristaux d'albite, en association avec gmelinite, neptunite, analcime, gonnardite, lovdarite, trona(?) et opale(?). La nabesite formes des aggrégats de minces cristaux en plaquette parallèles ou subparallèles; les cristaux individuels montrent les pinacoïdes {100}, {010}, {001}, ainsi que {111} et {111}, tous deux sphénoïdes, et varient entre 0.05 × 0.5 × 0.5 et 0.2 × 5 × 5 mm en taille. Il s'agit d'un minéral incolore et transparent, dont la rayure est blanche, et l'éclat, vitreux. La dureté de Mohs est entre 5 et 6. C'est un minéral cassant qui montre un bon clivage sur {110} et {001}, et la fracture est inégale. La nabesite est biaxe négative, avec n_α = 1.499(1), n_β = 1.507(1) et n_γ = 1.511(1), $2V_\alpha$ mesuré de 65(5)°, $2V_\alpha$ calculé de 70°, avec $X = a$, $Y = c$ et $Z = b$. La densité mesurée est égale à 2.16(2) g/cm^3, tandis que la densité calculée est égale à 2.21 et 2.22 g/cm^3 pour un volume *V* dérivé à partir de données en diffraction X sur poudre et sur cristal unique, respectivement. Les données obtenues par microsonde électronique, par microscopie

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électronique à balayage et par ébauche de la structure cristalline mènent à la composition suivante: Na_2O 13.8, K_2O 0.34, BeO 6.26, CaO 0.13, SiO_2 62.4, H_2O 18.05, total 100.98% (base pondérale). La formule idéale est $Na_2BeSi_4O_{10}•4H_2O$. Les raies les plus intenses du spectre de diffraction, méthode des poudres [*d* en Å (I) (*hkl*)] sont: 6.11(80)(111), 5.97(100)(002), 3.09(70)(310), 3.06(50)(222) et 2.988(60)(311). Les paramètres réticulaires, affinés à partir d'un spectre de diffraction sur poudre, sont: *a* 9.722(1), *b* 10.142(1), *c* 12.030(1) Å, *V* = 1186.2 Å^3. La structure a été déterminée par diffraction X sur cristal unique. La nabesite cristallise dans le système orthorhombique, groupe spatial $P2_12_12_1$, *a* 9.748(1), *b* 10.133(1), *c* 11.954(2) Å, *V* 1180.8(2) Å^3, *Z* = 4. Dans l'affinement, nous avons utilisé un total de 5704 réflexions uniques (à 293 K) pour atteindre un facteur de concordance *R*1 final de 0.028 (*wR*2 = 0.078). Les tétraèdres [SiO_4] sont agencés en feuillets contenant une combinaison d'anneaux à quatre et à huit membres, interconnectés *via* les tétraèdres [BeO_4] pour donner une trame, avec un agencement spiro-5 comme unité secondaire. Des canaux contiennent les atomes de sodium, à coordinence octaédrique, et des molécules de H_2O ayant un système de liaisons hydrogène bien établi. La nabesite est une zéolite qui présente une nouvelle sorte de trame; la densité de cette trame est de 16.94 *T* / 1000 Å^3. Les ressemblances à la structure cristalline de la weinebeneïte sont évidentes.

(Traduit par la Rédaction)

Mots-clés: nabesite, nouvelle espèce minérale, structure cristalline, zéolite, complexe alcalin d'Ilímaussaq, Groënland.

Introduction

Deep carmine red tugtupite, the Greenland gemstone par excellence, was found in 1965 in a limited number of rather complex albitites, on the Kvanefjeld Plateau, in the northwesternmost part of the Ilímaussaq alkaline complex, South Greenland. Relentless searches for this gemstone have left the landscape severely scarred and spotted with pits and covered by extensive piles of boulders, piles that have proven to be a real mineralogical treasure trove. The nabesite was found in one of these piles by two of the authors (OVP and GN) during a mineralogical excursion in the summer of 1999, and first mentioned as an "unidentified, platy, probably tetragonal mineral partly altered to opal" by Petersen *et al.* (2002).

The mineral is named after its chemical composition, $Na_2BeSi_4O_{10}•4H_2O$. The mineral and the mineral name were approved by the Commission on New Minerals and Mineral Names of IMA, September 2000, IMA #2000–024. Cotype material is preserved in the collections of the Geological Museum, Copenhagen, Denmark and the Natural History Museum, Vienna, Austria.

Occurrence

The tugtupite-bearing albitites on the Kvanefjeld Plateau are traceable over a distance of less than 100 meters, cutting augite syenite of the marginal zone and the roof of the complex. Associated minerals include aegirine, analcime, beryllite, bertrandite, chkalovite, epistolite, galena, manganoan pectolite ("schizolite"), microcline, Na-komarovite, neptunite, pyrochlore, sphalerite and tugtupite. Petrographic details of these albitites are given by Sørensen *et al.* (1971).

In many places, these albitites have proven to be rich in crystal-lined cavities. By far most of the crystals in the cavities consist of albite, in several generations and of highly variable habit, the last generation including Baveno-right twins of an odd wedge-shaped habit (Petersen *et al.* 2001). In addition to nabesite, distinct prismatic crystals of creamy gmelinite with brilliantly shiny pyramids, well-developed crystals of neptunite, perfect, colorless, transparent crystals of analcime, whitish gonnardite as sprays, fans and balls, very small off-white wagon-wheel aggregates of lovdarite (Petersen *et al.* 2002) and an as yet unidentified white, extremely soft, partly fibrous phase, presumed to be trona, are found in these cavities.

Morphology, General Physical and Optical Properties

Two crystals were selected and measured on a two-circle goniometer. The faces and forms were identified by comparing the stereographic projection obtained showing the faces present with a stereographic projection of possible faces and forms, constructed using the unit-cell parameters. The orientation of the first projection was determined by the use of a precession photograph. The indices and form names given here and in Figure 1 are for the crystal class 222 (inferred from the structural study); the forms identified are: the pinacoids {100}, {010} and {001}, and {111} and $\{\bar{1}11\}$, both sphenoids. The crystals are distinctly platy on {001}; the equal development of the two remaining pinacoids

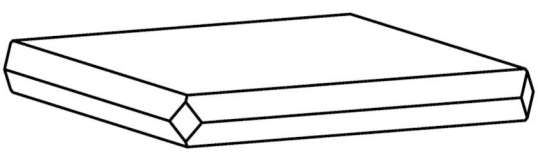

FIG. 1. Drawing of an idealized crystal of nabesite. The distinct platy crystal shows the forms {100}, {010}, {001}, {111} and $\{\bar{1}11\}$; the equal development of the two sphenoids makes the crystals seem holosymmetrical.

and, in particular, of the two sphenoids makes the crystals of nabesite seem holosymmetrical. Figure 1 shows a drawing of an idealized crystal.

Nabesite forms aggregates of thin platy crystals, in parallel or subparallel orientation, up to 5 × 10 × 10 mm in size; the individual crystals range in size from 0.05 × 0.5 × 0.5 to 0.2 × 5 × 5 mm. It is colorless, transparent, has a white streak, and the luster is vitreous. No fluorescence under ultraviolet light was observed. The Mohs hardness is 5–6; nabesite is brittle. The crystals show good cleavage on {110} and {001}, and the fracture is uneven. The density, determined by suspending the material in heavy liquids, is 2.16(2) g/cm^3; the density calculated from the empirical formula, and the unit-cell parameters derived from the X-ray powder diffraction and from single-crystal diffraction data, are, respectively, 2.21 and 2.22 g/cm^3, $Z = 4$.

Many of the nabesite crystals are partly covered by, partly or completely altered to, a white, X-ray-amorphous substance, a SEM–EDS analysis of which shows nothing but Si. Some of the partly altered crystals (Fig. 2) show this alteration as advancing along closely spaced planes parallel to {100} and, to a lesser extent, also {010}, at first creating an impression of two directions of poor cleavage or parting. We tentatively suggest that the substance is opal; attempts to determine the index of refraction by conoscopic refractometry (Micheelsen 1975), however, resulted in a value of 1.483(5), *i.e.*, a little too high for opal.

Nabesite is biaxial, optically negative with $2V_\alpha$ = 65(5)° as determined by orthoscopic spindle-stage technique and the program EXCALIBR II (Bloss 1981, Bartelmehs *et al.* 1992). The following indices of refraction for λ = 589 nm were determined by means of the microrefractometer spindle-stage, using calcite as refractometer crystal (Medenbach 1985) and under the application of the λ – T variation method: $n_\alpha = 1.499(1)$, $n_\beta = 1.507(1)$, $n_\gamma = 1.511(1)$. $2V_\alpha$ calculated was found to be 70°.

The orientation of the indicatrix relative to the unit cell as determined from precession photographs is: $X = a$, $Y = c$ and $Z = b$. Nabesite is colorless and shows no dispersion.

Chemical Composition

The chemical composition of nabesite, given in Table 1, was established by means of the electron microprobe (EMP) technique (K, Ca and Si) and by scanning electron microscopy with an energy-dispersion spectrometer SEM–EDS (Na). The amounts of Be and

TABLE 1. CHEMICAL COMPOSITION OF NABESITE

Na_2O wt.%	13.8	13.6 – 14.0	SiO_2	62.4	61.7 – 63.5
K_2O	0.34	0.32 – 0.36	H_2O	(18.05)	
BeO	(6.26)				
CaO	0.13	0.11 – 0.14	Total	(100.98)	

The composition reported is the average result of three electron-microprobe analyses. The amount of Na_2O was determined by SEM–EDS; the amounts of BeO and H_2O are calculated from the ideal formula, derived from the crystal-structure analysis.

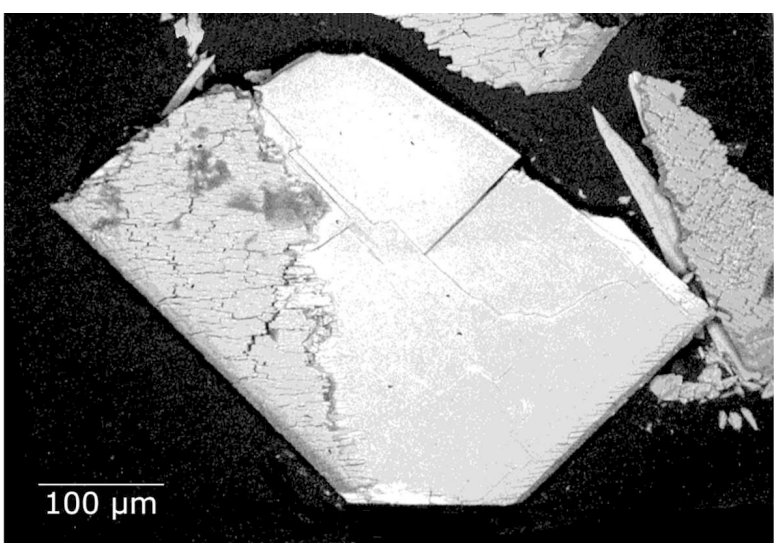

FIG. 2. Crystal of nabesite from the Ilímaussaq alkaline complex, South Greenland exhibiting partial alteration advancing along closely spaced planes parallel to {100} and, to a lesser extent, {010}. SEM image, secondary electron mode.

H_2O were calculated on the basis of results derived from the refinement of the crystal structure. The EMP analyses were performed on an ARL–SEMQ electron microprobe at 15 kV and 15 nA sample current (measured on benitoite) using the following standards: orthoclase ("adularia") (K), augite (Ca) and albite (Si). Plots of a series of 2-second counts in a count rate *versus* time diagram for EMP analyses of nabesite showed a significant decrease in Na counts with time, whereas the Si count rate was stable. On the other hand, SEM–EDS analyses gave constant Si/Na values for different counting times and were therefore chosen as the analytical method for Na. All analyses were carried out on a JEOL JSM–6400 scanning electron microscope equipped with a KEVEX energy-dispersion system and were performed as "standardless" analyses, with results normalized to a total of 100%. The Na content was determined by recalculating the corresponding EDS values using the microprobe-established values of Si.

The empirical formula, calculated on the basis of a total number of 10 anions in the anhydrous part, is: $(Na_{1.74}K_{0.03}Ca_{0.01})_{\Sigma 1.78}Be_{0.98}Si_{4.06}O_{10}\cdot 3.92H_2O$. The ideal formula of nabesite is: $Na_2BeSi_4O_{10}\cdot 4H_2O$.

The compatibility index $1-(K_P/K_C)$ is equal to 0.010 and 0.014 calculated using the unit-cell parameters derived from the X-ray powder-diffraction data and the unit-cell parameters derived from the single-crystal study, respectively. The compatibility is superior (Mandarino 1981).

X-Ray Diffraction and Crystal-Structure Determination

X-ray powder-diffraction data of nabesite, collected with a 114.6 mm Gandolfi camera and Cu$K\alpha$ radiation, are given in Table 2. Nabesite is orthorhombic; the unit-cell parameters refined from the powder data are: *a* 9.722(1), *b* 10.142(1), *c* 12.030(1) Å, *V* 1186.2 Å^3.

TABLE 2. X-RAY POWDER-DIFFRACTION DATA FOR NABESITE

I	$d_{meas.}$(Å)	$d_{calc.}$(Å)	*h k l*	*I*	$d_{meas.}$(Å)	$d_{calc.}$(Å)	*h k l*
5	7.76	7.754	0 1 1	70	3.09 D	3.087	3 1 0
10	7.08	7.018	1 1 0			3.086	1 3 1
80	6.11 B	6.062	1 1 1	50	3.06	3.031	2 2 2
100	5.97	6.015	0 0 2			3.008	0 0 4
35	5.07	5.071	0 2 0			(2.993	1 2 3)
10	4.90	4.861	2 0 0	60	2.988 D	2.990	3 1 1
10	4.67	4.673	0 2 1	30	2.828	2.820	1 3 2
30	4.60	4.567	1 1 2	30	2.747	2.764	1 1 4
10	4.14	4.119	2 1 1			2.746	3 1 2
5	3.69	3.707	1 0 3	25	2.641	2.641	2 2 3
45	3.46	3.482	1 1 3	15	2.550	2.558	2 0 4
10	3.41	3.369	2 2 1	20	2.495	2.498	1 3 3
10	3.19	3.193	1 3 0	15	2.295	2.296	3 3 1
		(3.093	2 0 3)	10	2.206	2.210	2 4 1
				10	2.151	2.154	3 1 4

B: broad, D: double. ( ): I ≈ 0 in the calculated diagram.

Precession photographs with the 12.03 Å *c*-axis as the precession axis and the 9.72 Å *a*-axis as the dial axis mainly served to determine the orientation of the indicatrix relative to the unit cell.

Single-crystal X-ray data of nabesite were measured with a Nonius Kappa CCD diffractometer at 100 K, 293 K, as well as at 300 K (after partial dehydration). Data collections were performed with a 2° rotation width of the frames. The measurement at 300 K was made under a permanent flow of dry nitrogen gas starting after 12 hours waiting time. Within these 12 hours, the quality of the diffraction pattern and the unit-cell dimensions were checked several times until no further changes were observed.

Throughout the text, details refer to the room-temperature measurement (293 K) unless explicitly mentioned. A chip of an unaltered crystal, 0.24 × 0.20 × 0.08 mm in size, was cut from a larger specimen. Crystal data as well as experimental details are compiled in Table 3. The measured intensities were corrected for Lorentz and polarization effects. The crystal structure of nabesite was solved by direct methods (SHELXS–97, Sheldrick 1997a) and subsequent Fourier and difference-Fourier syntheses. The structure refinement by full-matrix least-squares techniques on F^2 was made with SHELXL–97 (Sheldrick 1997b). The positions of the hydrogen atoms of the H_2O molecules (OW1–OW4) were finally located by difference-Fourier maps. Atomic coordinates and isotropic temperature-factors for all hydrogen atoms could be refined (for the H_2O molecule of OW3, constraints were applied for OW3–H and H–H to maintain the correct geometry).

TABLE 3. CRYSTAL DATA AND DETAILS OF THE INTENSITY MEASUREMENTS AND STRUCTURE REFINEMENTS FOR NABESITE

	T = 100 K	T = 293 K	T = 300 K
Crystal system, space group	orthorhombic, $P2_12_12_1$		
a (Å)	9.723(1)	9.748(1)	9.700(7)
b (Å)	10.144(1)	10.133(1)	10.028(7)
c (Å)	11.899(1)	11.954(2)	11.977(8)
V (Å^3)	1173.6(2)	1180.8(2)	1165.0(14)
Z	4	4	4
D_{calc} (g/cm^3)	--	2.22	--
μ(Mo$K\alpha$) (cm^{-1})	6.6	6.6	--
Atmosphere	--	--	N_2
Extinction coefficient	0.0003(7)	0.007(1))	--
$2\theta_{max}$ (°)	72.6	72.6	53.0
Unique data set	5484	5704	2220
Data with $F_o > 4\sigma(F_o)$	5061	5443	1274
Variables / restraints	223 / 2	223 / 2	172 / 0
Flack parameter	0.09(8)	–0.05(8)	0.2(8)
*R*1 [for $F_o > 4\sigma(F_o)$]	0.028	0.028	0.117
*wR*2 [for all F_o^2]	0.076	0.078	0.356
a; b	0.04; 0.5	0.04; 0.5	0.08; 35.0
$\rho_{min\,/\,max}$ (eÅ^{-3})	–0.69/0.68	–0.66 / 0.44	–1.08/1.03
Crystal–detector distance (mm)	35	28	35
Number of sets; frames	10; 510	10; 416	4; 223
Exposure time (s) / frame	70	70	55

$R1 = \Sigma F_o - F_c / \Sigma F_o$, $wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma wF_o^4]^{1/2}$, $w = 1 / [\sigma^2(F_o^2) + (a \times P)^2 + b \times P]$, $P = \{[\max of (0 or F_o^2)] + 2F_c^2\} / 3$.

The structure parameters of nabesite are compiled in Table 4; selected interatomic distances and bond angles, including the proposed scheme of hydrogen bonds, are given in Tables 5 and 6. Respective information on measurements performed at 100 and 300 K can be obtained from the authors upon request. Tables of structure factors for all three data-sets and tables of atom coordinates for the refinements at 100 and 300k are available from the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2.

Description and Discussion of the Structure

The framework structure of nabesite is built up of corner-sharing [XO_4] groups, the central *X* ion being located at five distinct crystallographic sites. The structure refinement unambiguously proves that the Be and Si atoms are ordered among these sites (*i.e.*, one Be and four Si positions). The [SiO_4] tetrahedra form sheets containing a combination of 4- and 8-membered rings, parallel to (001) at $z/c \approx 0.0$ and 0.5 (Fig. 3a). These sheets are linked to each other *via* [BeO_4] groups at $z/c \approx 0.25$ and 0.75 (Fig. 3b), to give a spiro-5 arrangement (Fig. 4) as secondary building unit (*cf.* Baerlocher *et al.* 2001). Interstices within the framework are occupied by octahedrally coordinated sodium atoms (Na1, Na2) and H_2O molecules of OW1–4 (Fig. 5).

The [SiO_4] tetrahedra have mean Si–O bond lengths within 1.618–1.621 Å, and the [BeO_4] tetrahedron has a mean Be–O bond length of 1.643 Å, all values being in good agreement with data in the literature (1.623 and 1.634 Å, respectively, *cf.* Baur 1981). The [SiO_4] tetrahedra show larger distortions of bond angles and bond lengths than the [BeO_4] group. This finding may indicate that the [SiO_4] tetrahedra are much more rigidly interconnected within the sheets parallel to (001). Upon cooling to 100 K, the *c* cell edge decreases (–0.46%), whereas *a* and *b* change by –0.26% and +0.11%, respectively (Table 3).

The sodium atoms (Na1, Na2) each have a distorted octahedral coordination to three oxygen atoms of the H_2O molecules and three oxygen atoms of the framework. Both polyhedra are combined *via* a common edge (OW1–OW2) to a dimeric group. The Na–O distances are in the range 2.32–2.71 Å; further oxygen atoms are more than 3.18 Å apart.

TABLE 4. ATOMIC COORDINATES AND ANISOTROPIC DISPLACEMENT PARAMETERS FOR NABESITE

Atom	*x*	*y*	*z*	$U_{eqv/iso}$	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Na1	0.02823(8)	0.19660(8)	0.81506(7)	0.02878(16)	0.0224(3)	0.0304(4)	0.0335(4)	-0.0083(3)	-0.0043(3)	0.0052(3)
Na2	0.37372(12)	0.25369(9)	0.73922(9)	0.0447(2)	0.0554(6)	0.0330(4)	0.0456(5)	0.0029(4)	-0.0111(5)	0.0044(4)
Be	0.24232(15)	0.26224(16)	0.25678(12)	0.0084(2)	0.0104(6)	0.0078(6)	0.0070(6)	0.0003(4)	-0.0025(5)	-0.0009(4)
Si1	0.08393(3)	0.35478(3)	0.06419(3)	0.00750(6)	0.00767(12)	0.00662(12)	0.00820(12)	0.00026(10)	-0.00143(9)	0.00092(10)
Si2	0.39961(3)	0.36283(3)	0.44722(3)	0.00765(6)	0.00782(12)	0.00677(12)	0.00835(12)	-0.00044(10)	-0.00094(9)	-0.00128(9)
Si3	0.29128(3)	0.14866(3)	0.03408(3)	0.00839(6)	0.00822(12)	0.00770(12)	0.00926(12)	-0.00077(10)	0.00010(9)	0.00122(10)
Si4	0.20023(3)	0.14856(3)	0.47842(3)	0.00781(6)	0.00819(12)	0.00702(12)	0.00821(12)	0.00068(10)	-0.00033(9)	-0.00160(10)
O1	0.11930(10)	0.34407(10)	0.19374(7)	0.01217(15)	0.0143(4)	0.0137(4)	0.0085(3)	-0.0007(3)	-0.0033(3)	0.0047(3)
O2	0.12092(13)	0.49694(9)	0.01041(9)	0.01716(19)	0.0232(5)	0.0085(4)	0.0198(4)	0.0054(3)	0.0002(4)	-0.0008(3)
O3	-0.07946(10)	0.32732(10)	0.04934(9)	0.01433(17)	0.0082(3)	0.0194(4)	0.0153(4)	0.0012(3)	-0.0033(3)	0.0002(3)
O4	0.16731(10)	0.24433(9)	-0.00928(8)	0.01126(15)	0.0130(3)	0.0110(3)	0.0098(3)	-0.0017(3)	-0.0020(3)	0.0056(3)
O5	0.34741(10)	0.36353(9)	0.32118(8)	0.01214(15)	0.0147(4)	0.0123(3)	0.0094(3)	0.0009(3)	-0.0039(3)	-0.0040(3)
O6	0.56197(10)	0.32609(11)	0.44915(9)	0.01601(18)	0.0076(3)	0.0219(4)	0.0185(4)	-0.0028(4)	-0.0024(3)	0.0012(3)
O7	0.31580(9)	0.25353(9)	0.52237(7)	0.01135(15)	0.0133(4)	0.0102(3)	0.0105(3)	0.0011(3)	-0.0013(3)	-0.0054(3)
O8	0.32791(10)	0.17820(10)	0.16101(8)	0.01294(16)	0.0143(4)	0.0156(4)	0.0089(3)	-0.0030(3)	-0.0028(3)	0.0043(3)
O9	0.24094(11)	-0.00340(8)	0.01423(9)	0.01378(17)	0.0161(4)	0.0064(3)	0.0189(4)	-0.0025(3)	0.0021(3)	0.0000(3)
O10	0.17608(11)	0.15933(10)	0.34733(8)	0.01483(17)	0.0207(4)	0.0153(4)	0.0085(3)	0.0024(3)	-0.0033(3)	-0.0078(3)
OW1	0.22056(17)	0.07549(13)	0.76168(11)	0.0277(3)	0.0474(7)	0.0182(5)	0.0176(5)	-0.0026(4)	-0.0078(5)	0.0091(5)
OW2	0.16099(19)	0.37520(14)	0.73814(13)	0.0316(3)	0.0475(8)	0.0203(5)	0.0270(6)	-0.0036(5)	-0.0055(6)	0.0033(6)
OW3	-0.05881(17)	0.02080(17)	0.94934(15)	0.0379(3)	0.0354(8)	0.0387(8)	0.0396(9)	-0.0047(7)	-0.0076(7)	-0.0034(6)
OW4	0.47439(19)	0.44438(17)	0.80888(15)	0.0394(4)	0.0399(8)	0.0361(8)	0.0421(8)	0.0176(7)	-0.0003(7)	0.0086(7)
H1	0.249(4)	0.009(4)	0.807(3)	0.066(10)						
H2	0.209(4)	0.049(4)	0.689(3)	0.067(11)						
H3	0.171(3)	0.442(3)	0.759(3)	0.045(8)						
H4	0.095(4)	0.383(4)	0.699(3)	0.059(10)						
H5	-0.077(3)	0.029(3)	1.0225(18)	0.047(9)						
H6	0.034(2)	0.011(4)	0.959(4)	0.102(15)						
H7	0.446(4)	0.527(4)	0.788(3)	0.074(12)						
H8	0.554(4)	0.404(4)	0.765(3)	0.075(12)						

The anisotropic displacement parameter is defined as: $exp(-2\pi^2 \Sigma_i \Sigma_j U_{ij} h_i h_j a^*_i a^*_j)$. Temperature: 293 K.

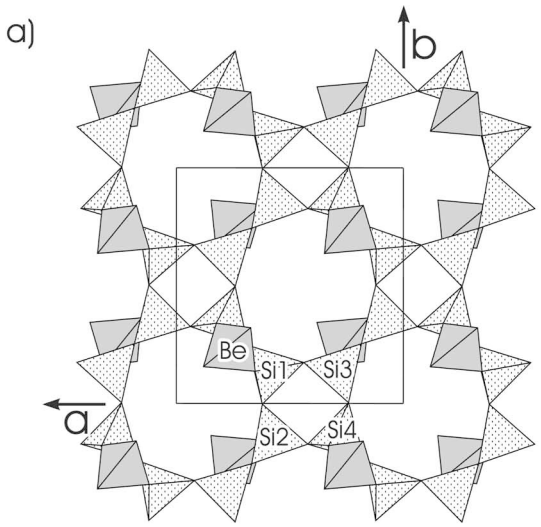

FIG. 3. Single sheet in nabesite in projections parallel (a) [001] and (b) [010]. All structure drawings are made with the program ATOMS (Dowty 1999).

Four distinct H_2O molecules exist in the structure of nabesite. Two of them (OW1, OW2) bridge both Na1 and Na2 along [100], whereas OW3 and OW4 belong to the coordination sphere of only one sodium atom. The system of hydrogen bonds is given in Table 6. The calculation of bond-valence sums v for oxygen atoms (Table 7, according to Brese & O Keeffe 1991, excluding contributions of hydrogen atoms) corroborates the proposed model. Non-acceptor oxygen atoms are in the range 2.00–2.08 *vu* (valence units), acceptor atoms between 1.60 and 1.94 *vu*. The donor atoms OW3 and OW4, which are only bound to one sodium atom each, further act as acceptor atoms of hydrogen bonds. The non-acceptor atoms are two-coordinated (O2: Si–O2–Si = 159.66°; O6: Si–O6–Si = 141.26°) or almost planar and three-coordinated (O3, O4, O7), whereas all other oxygen atoms are in distorted tetrahedral coordination if one also takes the hydrogen atoms into account.

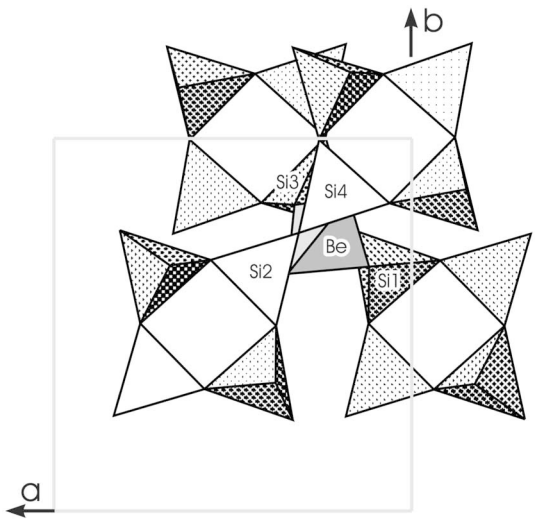

FIG. 4. Detail of the structure of nabesite illustrating the spiro-5 arrangement around a [BeO_4] tetrahedron.

TABLE 5. SELECTED INTERATOMIC DISTANCES [Å], ANGLES [°] AND BOND-VALENCE SUMS [*vu*]* FOR NABESITE

Si1-O1	1.5902(9)	1.10 *vu*	Si4-O10	1.5884(10)	1.10 *vu*
Si1-O2	1.6181(10)	1.02	Si4-O6	1.6223(10)	1.00
Si1-O3	1.6266(10)	0.99	Si4-O9	1.6357(10)	0.97
Si1-O4	1.6385(9)	0.96	Si4-O7	1.6360(9)	0.97
<Si1-O>	<1.618>	4.07	<Si4-O>	<1.621>	4.04
O1-Si1-O2	113.54(5)		O10-Si4-O6	113.11(6)	
O1-Si1-O3	107.87(5)		O10-Si4-O9	111.83(6)	
O2-Si1-O3	109.09(6)		O6-Si4-O9	107.10(6)	
O1-Si1-O4	111.58(5)		O10-Si4-O7	111.98(5)	
O2-Si1-O4	106.53(6)		O6-Si4-O7	107.32(5)	
O3-Si1-O4	108.08(5)		O9-Si4-O7	105.02(5)	
Si2-O5	1.5902(9)	1.10 *vu*	Be-O10	1.6358(18)	0.50 *vu*
Si2-O2	1.6217(10)	1.01	Be-O1	1.6412(17)	0.50
Si2-O6	1.6260(10)	0.99	Be-O5	1.6418(17)	0.49
Si2-O7	1.6436(9)	0.95	Be-O8	1.6528(18)	0.48
<Si2-O>	<1.620>	4.05	<Be-O>	<1.643>	1.97
O5-Si2-O2	113.45(5)		O10-Be-O1	109.72(10)	
O5-Si2-O6	109.03(6)		O10-Be-O5	109.54(9)	
O2-Si2-O6	108.31(6)		O1-Be-O5	110.82(11)	
O5-Si2-O7	111.21(5)		O10-Be-O8	109.21(11)	
O2-Si2-O7	105.93(5)		O1-Be-O8	108.13(9)	
O6-Si2-O7	108.77(6)		O5-Be-O8	109.39(10)	
Si3-O8	1.5873(10)	1.10 *vu*	Na1-OW1	2.3298(17)	0.24 *vu*
Si3-O3	1.6252(10)	1.00	Na1-O8	2.3462(13)	0.23
Si3-O4	1.6337(9)	0.97	Na1-OW2	2.4073(19)	0.19
Si3-O9	1.6344(9)	0.97	Na1-O5	2.4760(13)	0.16
<Si3-O>	<1.620>	4.05	Na1-OW3	2.544(2)	0.13
			Na1-O4	2.5458(12)	0.13
O8-Si3-O3	112.58(5)		<Na1-O>	2.442	1.08
O8-Si3-O4	110.97(5)				
O3-Si3-O4	106.85(5)		Na2-OW4	2.322(2)	0.24 *vu*
O8-Si3-O9	112.59(6)		Na2-OW1	2.358(2)	0.22
O3-Si3-O9	106.55(5)		Na2-OW2	2.412(2)	0.19
O4-Si3-O9	106.94(6)		Na2-O7	2.6529(14)	0.10
			Na2-O3	2.6965(15)	0.09
			Na2-O1	2.7119(15)	0.08
			<Na2-O>	2.526	0.93

* Calculation of bond-valence sums according to Brese & O'Keeffe (1991); the contributions of the hydrogen atoms were not taken into account.

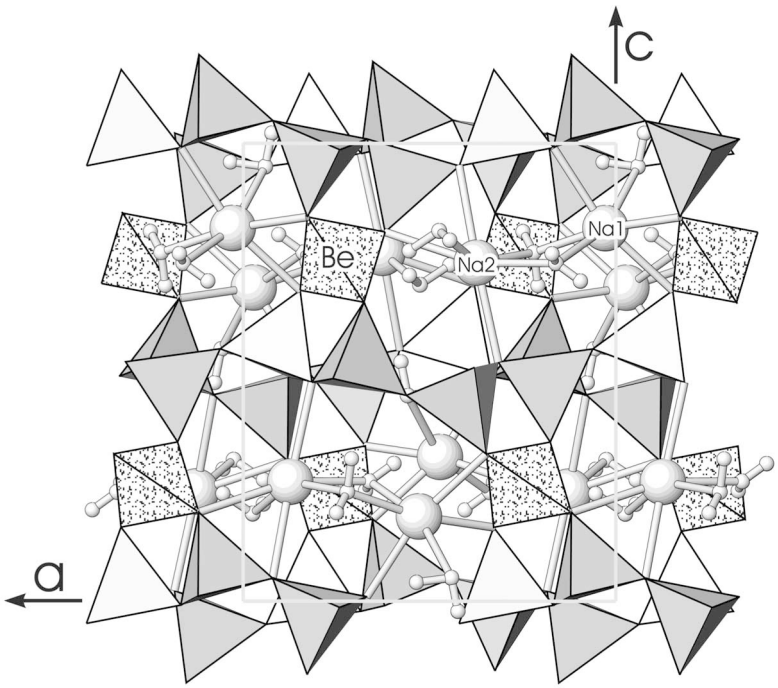

FIG. 5. The crystal structure of nabesite projected along [010]. The sodium atoms are represented by large spheres, and the oxygen and hydrogen atoms of the H_2O groups, by small ones.

TABLE 6. SYSTEM OF HYDROGEN BONDS IN NABESITE

D–H	d(D–H)	D–H···A	d(D–A)	∠ (D–H···A)	H–D–H	∠ (H–D–H)
OW1-H1	0.91(4)	OW1-H1···O10	2.779	157.8	H1-OW1-H2	113(3)
OW1-H2	0.91(4)	OW1-H2···O9	3.070	159.8		
		OW1-H2···O8	2.877	116.2		
OW2-H3	0.73(3)	OW2-H3···O5	2.829	166.9	H3-OW2-H4	103(3)
OW2-H4	0.80(4)	OW2-H4···OW3	2.862	129.8		
OW3-H5	0.89(2)	OW3-H5···OW4	2.930	155.1	H5-OW3-H6	94(3)
OW3-H6	0.92(2)	OW3-H6···O9	3.033	169.3		
OW4-H7	0.92(4)	OW4-H7···O1	2.706	156.6	H7-OW4-H8	117(3)
OW4-H8	1.02(4)	OW4-H8···O10	2.908	165.7		

Distances in Å, angles in °.

TABLE 7. CALCULATION OF BOND-VALENCE SUMS v [*vu*]* FOR DONOR (D), ACCEPTOR (A) AND NON-ACCEPTOR (NON-A) OXYGEN ATOMS

D	v	A	v	Non-A	v
OW1	0.46	O1	1.68	O2	2.02
OW2	0.39	O5	1.75	O3	2.08
OW3	0.13	O8	1.81	O4	2.07
OW4	0.24	O9	1.94	O6	2.00
		O10	1.60	O7	2.02

vu: valence units.

Based on its crystal structure, nabesite may be classified as a zeolite with a new type of framework (*cf.* Baerlocher *et al.* 2001); the coordination sequences (numbers of neighboring *T* atoms linked through oxygen bridges, calculated for consecutive shells) are:

*T*1 (Be) 4 8 20 40 52 82 116 132 184 236

*T*2 (Si1–4) 4 9 19 40 55 80 115 138 183 229

The framework density is 16.94 *T* / 1000 Å^3(values for zeolites are reported in the range of 12.1 to 20.6: Baerlocher *et al.* 2001). Figures 6a–c illustrate the framework viewed along [001], [100] and [110], respectively.

Intersecting channels run along [110] and [$\bar{1}$10], which are occupied by the sodium atoms and the H_2O molecules. Owing to the small amount of unaltered nabesite available, no detailed dehydration and rehydration experiments were performed. Nevertheless, we can show that within 12 hours at 300 K under a stream of dry nitrogen, single crystals of nabesite lose a consider-

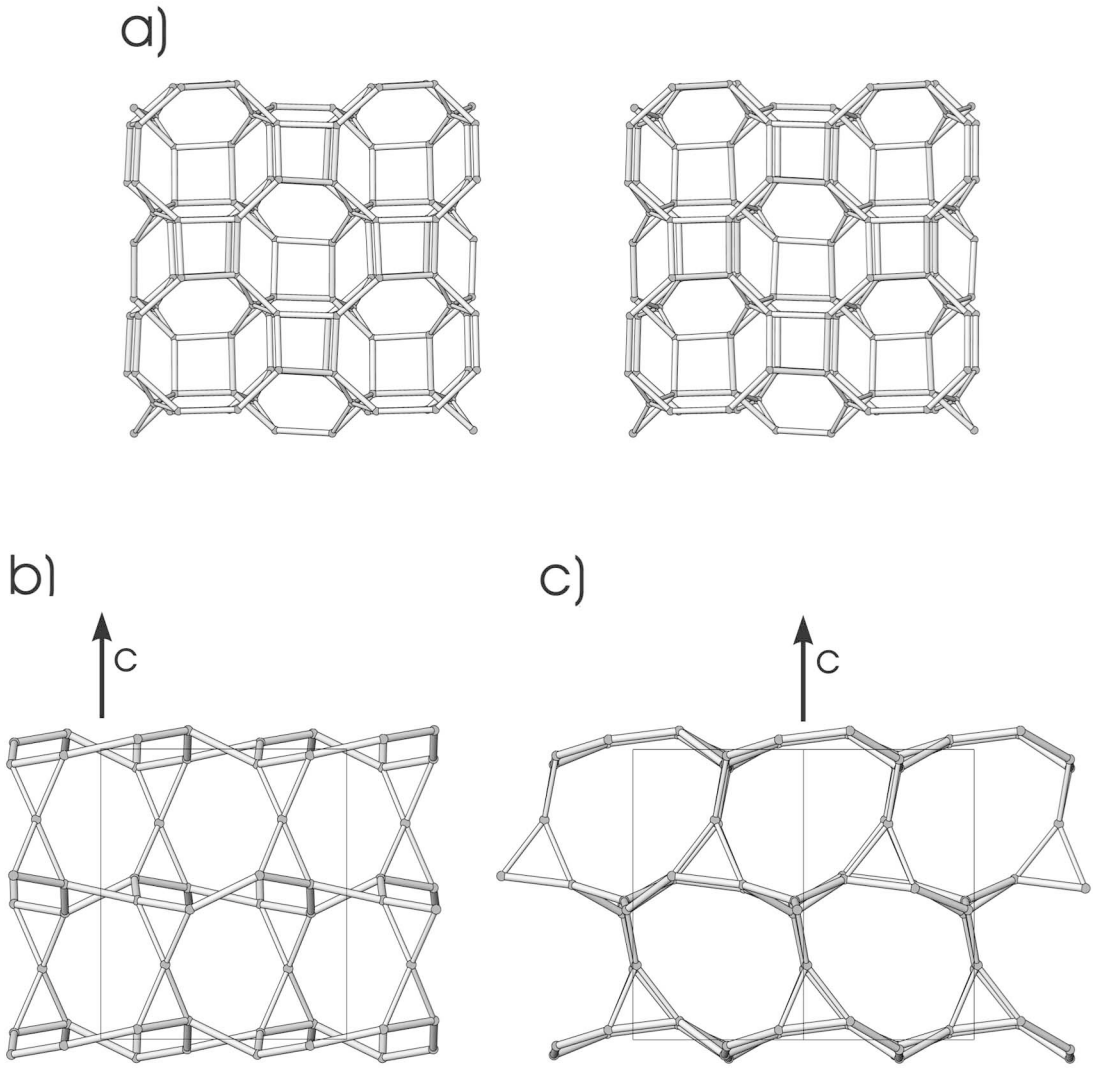

FIG. 6. Nabesite framework (a) in a stereographic view along [001], as well as in projections along (b) [100] and (c) [110].

able amount of H_2O. This loss is accompanied by a change of cell parameters (Table 3), especially a shrinkage of the *b* dimension, whereas the quality of the diffraction pattern steadily deteriorates. In spite of the inferior quality, data collection was performed under the above-mentioned conditions. The structure refinement proved that the more weakly bound H_2O molecules OW3 and OW4 had been released, causing a significant re-arrangement of the framework: the O7–Be–O4 axis of the spiro-5 group changes from 175.3° to 159.4° in the partially dehydrated structure. A unit-cell determination of the treated crystal, performed after one week at ambient conditions in air, again gave values close to those of unaltered nabesite but without completely reaching the original quality of the diffraction spots.

The structure of nabesite at low temperature (100 K) exhibits only minor changes with respect to the room-temperature arrangement.

Nabesite, $Na_2BeSi_4O_{10}•4H_2O$, is related to weinebeneite, $CaBe_3(PO_4)_2(OH)_2•4H_2O$ (Walter 1992). This mineral crystallizes in the monoclinic system, space group *Cc*, with cell constants of *a* 11.897, *b* 9.707, *c* 9.633 Å, β 95.76°. It too has spiro-5 secondary building units (Figs. 7a, b) and sheets formed from 4- and 8-

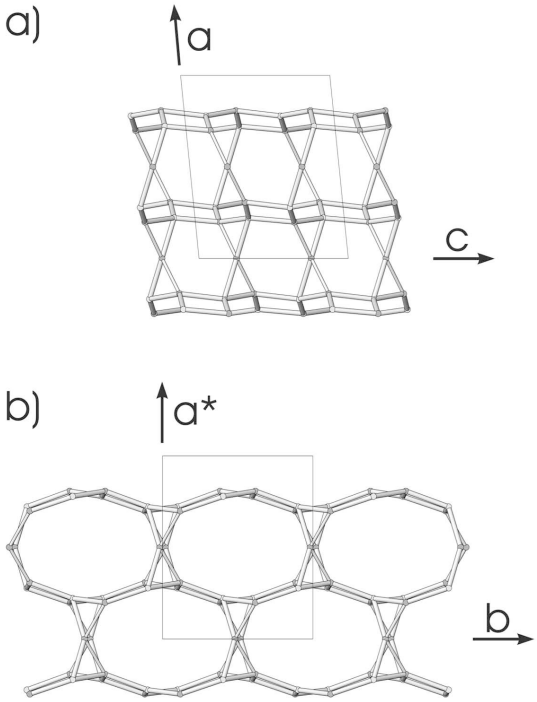

FIG. 7. The framework of weinebeneite in projections along (a) [010] and (b) [001].

membered rings, but with different coordination-sequences. Lovdarite, $K_4Na_{12}Be_8Si_{28}O_{72}$•$18H_2O$ (Merlino 1990) also contains spiro-5 groups, but not as secondary building units. This zeolite is orthorhombic, space group *Pma*2, with *a* 39.576, *b* 6.931, *c* 7.153 Å.

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